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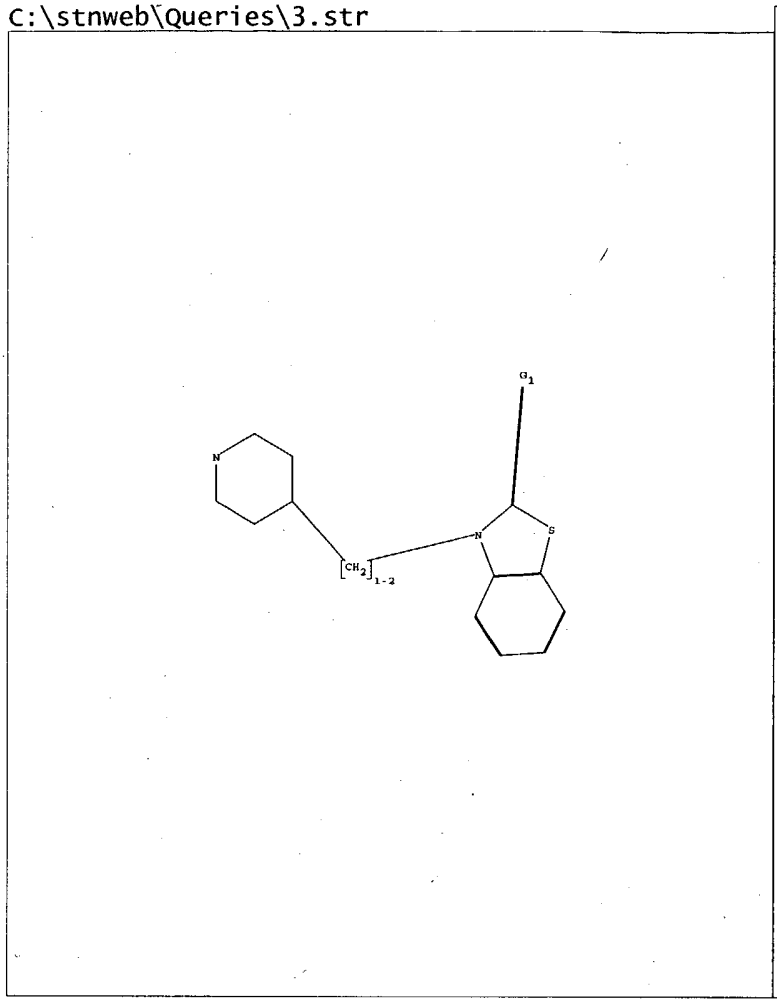

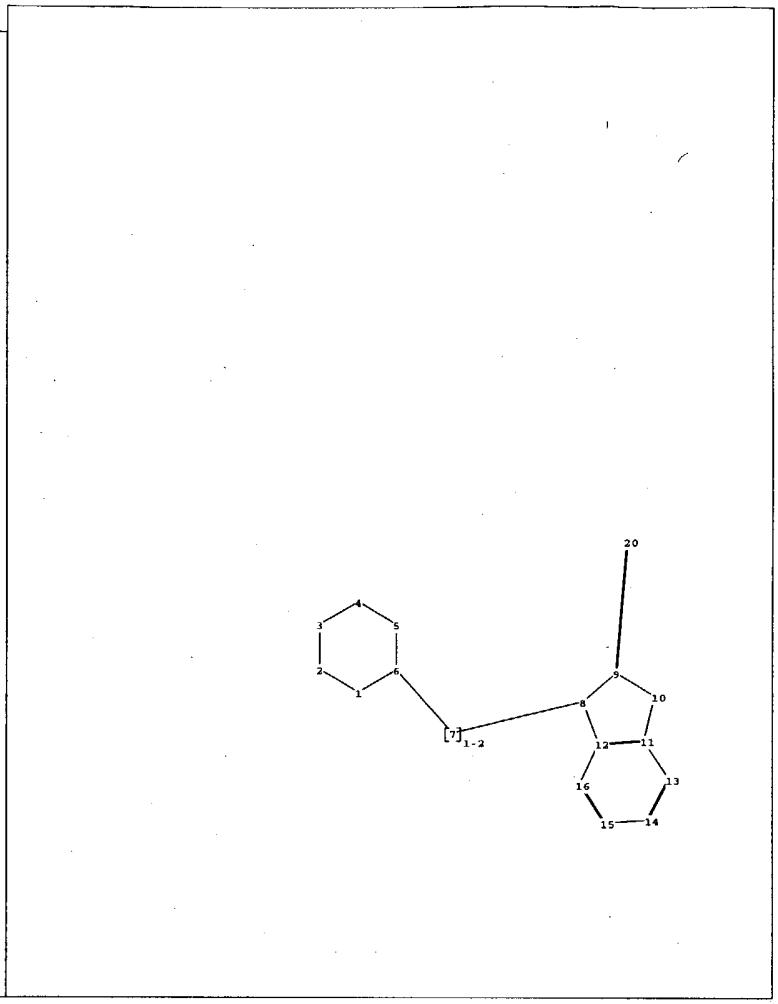

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7 20
ring nodes :
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ring bonds :
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exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-20
exact bonds :
6-7 7-8 9-10 10-11
normalized bonds :
11-12 11-13 12-16 13-14 14-15 15-16
isolated ring systems :
containing 1 : 8 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 20:CLASS

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* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  NOV 24   MSDS-CCOHS file reloaded
 NEWS  4  DEC 08   CABA reloaded with left truncation
 NEWS  5  DEC 08   IMS file names changed
 NEWS  6  DEC 17   DGENE: Two new display fields added
 NEWS  7  DEC 18   BIOTECHNO no longer updated
 NEWS  8  DEC 19   CROPU no longer updated; subscriber discount no longer
                   available
 NEWS  9  DEC 22   ABI-INFORM now available on STN
 NEWS 10  JAN 27   Source of Registration (SR) information in REGISTRY updated
                   and searchable
 NEWS 11  JAN 27   A new search aid, the Company Name Thesaurus, available in
                   CA/CAplus
 NEWS 12  FEB 05   German (DE) application and patent publication number format
                   changes
 NEWS 13  MAR 03   MEDLINE and LMEDLINE reloaded
 NEWS 14  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS 15  MAR 03   FRANCEPAT now available on STN
 NEWS 16  MAR 29   Pharmaceutical Substances (PS) now available on STN
 NEWS 17  MAR 29   WPIFV now available on STN
 NEWS 18  MAR 29   No connect hour charges in WPIFV until May 1, 2004
 NEWS 19  MAR 29   New monthly current-awareness alert (SDI) frequency in RAPRA

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
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FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004
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```

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7
DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> l1
L1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l1
L1 HAS NO ANSWERS
L1 STR
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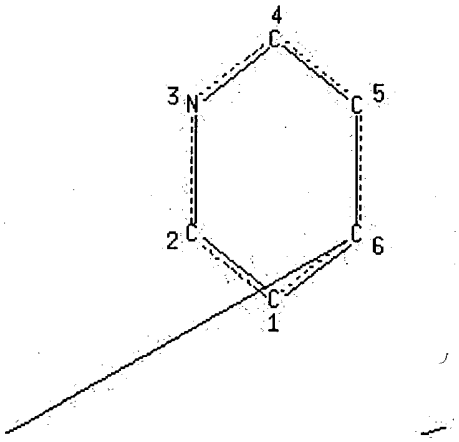
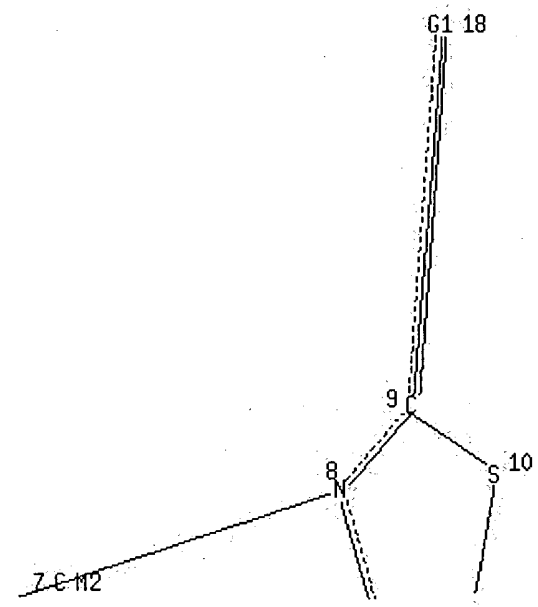
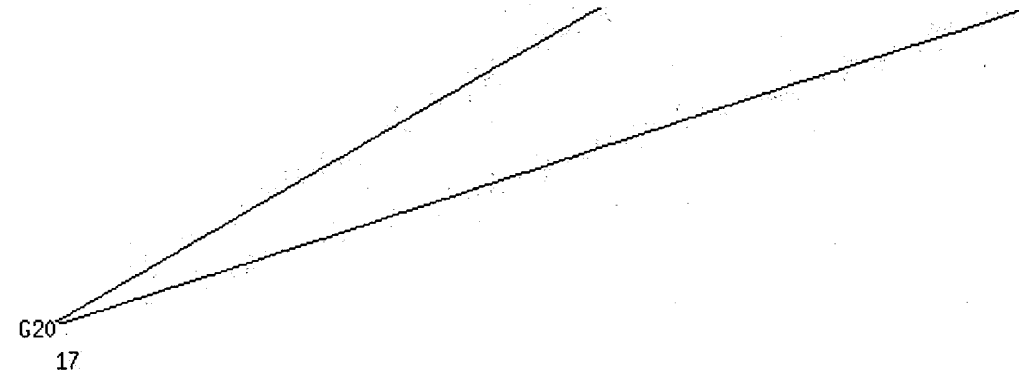


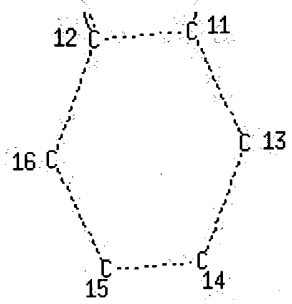
Page 1-A



Page 1-B



Page 2-A



Page 2-B

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NSPEC    IS C       AT   7
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NSPEC    IS R       AT   9
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE


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SAMPLE SEARCH INITIATED 15:25:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      5 TO ITERATE

100.0% PROCESSED       5 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            5 TO      234
PROJECTED ANSWERS:               2 TO      124

L2             2 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:25:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    104 TO ITERATE

100.0% PROCESSED     104 ITERATIONS                             45 ANSWERS
SEARCH TIME: 00.00.01

L3            45 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             157.10     157.31

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004
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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 7 L3

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69 ROCHER, J?/AU
L5 1 L4 AND ROCHER, J?/AU

=> **d l5, ibib abs fhitstr, 1**

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): **Rocher, Jean-Philippe**; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607 A	19971105
			WO 1998-JP4973 W	19981104

OTHER SOURCE(S): MARPAT 130:338102
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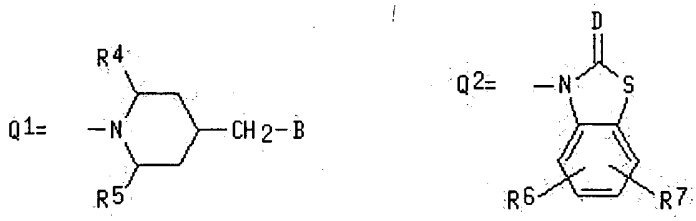


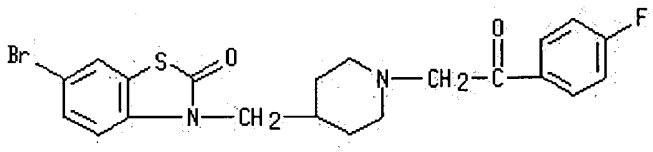
AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-05-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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     FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004
L1             STRUCTURE UPLOADED
L2               2 S L1
L3              45 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004
L4               7 S L3
L5               1 S L4 AND ROCHER, J?/AU

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            208 YAMABE, H?/AU
L6            1 L4 AND YAMABE, H?/AU

=> s l6 not l5
L7            0 L6 NOT L5

=> s l4 and chaki, h?/au
             74 CHAKI, H?/AU
L8            1 L4 AND CHAKI, H?/AU

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=> d l4, ibib abs fhitstr 1-7

L4   ANSWER 1 OF 7  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

ACCESSION NUMBER: 2001:372159 HCAPLUS

DOCUMENT NUMBER: 134:366868
TITLE: Preparation of benzothiazolines as neuropeptide Y receptor antagonists
INVENTOR(S): Sato, Yoshiya; Itani, Hiromichi; Tabuchi, Seiichiro; Sakata, Yoshihiko; Ohashi, Hiroko
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 88 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001139574	A2	20010522	JP 2000-296175	20000928

PRIORITY APPLN. INFO.: AU 1999-3093 A 19990928
OTHER SOURCE(S): MARPAT 134:366868
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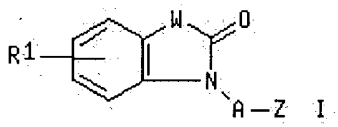
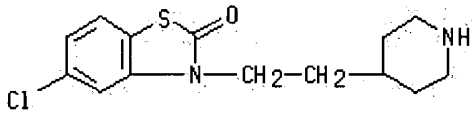


I

AB The title compds. I [R1 = H, halo; W = S, O; A = (CH2)n, etc.; n = 1 - 6; Z = (un)substituted N-contg. heterocyclic ring] are prepd. 1-[(5-Chloro-2-oxobenzothiazolin-3-yl)acetyl]piperidine-4-carboxylic acid 4-benzoylanilide showed IC100 of 10-7 M in a neuropeptide Y5 receptor binding assay.

IT **340179-40-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of benzothiazolines as neuropeptide Y receptor antagonists)

RN 340179-40-0 HCAPLUS
CN 2(3H)-Benzothiazolone, 5-chloro-3-[2-(4-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan

SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105

PRIORITY APPLN. INFO.: JP 1997-302607 A 19971105
WO 1998-JP4973 W 19981104

OTHER SOURCE(S): MARPAT 130:338102
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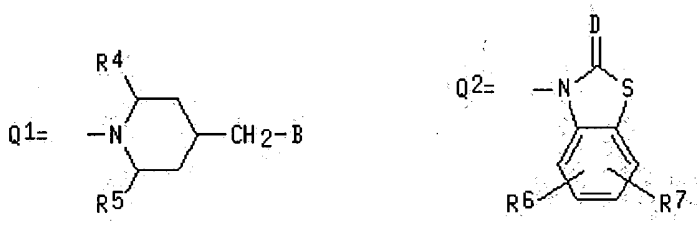


AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-

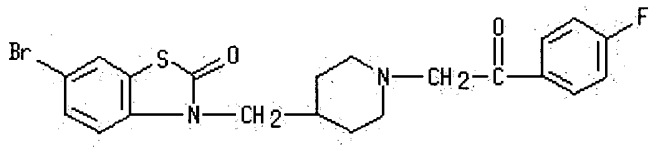
1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-05-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1993:191730 HCAPLUS
DOCUMENT NUMBER: 118:191730
TITLE: Preparation of benzothiazolinyltropolones for treatment of ischemia.
INVENTOR(S): McWhoster, William W.; Ito, Noriie; Ozawa, Kazunori; Kushida, Hiroshi; Nomura, Toshiharu; Kunihara, Mineo
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04247077	A2	19920903	JP 1991-56252	19910131
CA 2087004	AA	19920301	CA 1991-2087004	19910827
CA 2087004	C	19980421		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
AT 159251	E	19971115	AT 1991-917948	19910827
ES 2109276	T3	19980116	ES 1991-917948	19910827

NO 9300669	A	19930225	NO 1993-669	19930225
US 5594144	A	19970114	US 1995-442710	19950518
US 5703071	A	19971230	US 1995-443972	19950518

PRIORITY APPLN. INFO.:

JP 1990-229536	19900829
JP 1991-56252	19910131
JP 1991-39173	19910208
WO 1991-US5906	19910827
US 1993-975924	19930218

OTHER SOURCE(S): MARPAT 118:191730

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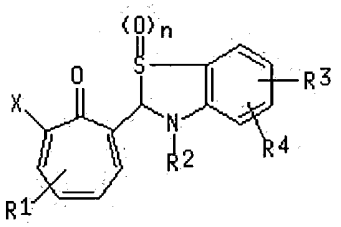


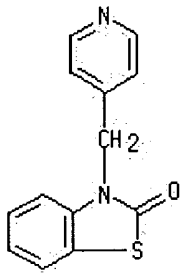
I

AB The title compds. [I; R1 = H, alkyl, (un)substituted aryl; R2 = H, alkyl, etc.; R3, R4 = H, alkyl, halo, OH, alkoxy, etc.; X = OH, alkoxy, etc.; n = 0, 1, 2] were prepd. E.g., 2-[(2-phenylethyl)amino]thiophenol (prepn. given) was refluxed with 2-methoxy-4-isopropyl-7-formyl-2,4,6-cycloheptatrien-1-one in toluene for 17 H to give I [X = MeO, R1 = 5'-iso-Pr, R2 = PhCH2CH2, R3 = R4 = H, n = 0]. At 0.1 mg/Kg i.p. this showed 50% effectiveness in counteracting brain ischemic rats in a learning study using rats.

IT **142224-26-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for benzothiazolinyltropolones for treatment of ischemia)

RN 142224-26-8 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1992:531223 HCAPLUS
DOCUMENT NUMBER:	117:131223
TITLE:	Preparation of heterocyclyltropolones as ischemia inhibitors
INVENTOR(S):	Ito, Noriie; Kunihara, Mineo; Kushida, Hiroshi; McWhoster, William W.; Nomura, Syunji; Ozawa, Kazunori; Taniguchi, Mikeo; Tsuzuki, Tazuo
PATENT ASSIGNEE(S):	USA

SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204338	A1	19920319	WO 1991-US5906	19910827
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US				
RW: AT, BE, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN				
JP 04120069	A2	19920421	JP 1990-229536	19900829
AU 9187203	A1	19920330	AU 1991-87203	19910827
AU 651629	B2	19940728		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
NO 9300669	A	19930225	NO 1993-669	19930225

PRIORITY APPLN. INFO.: JP 1990-229536 19900829
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WO 1991-US5906 19910827

OTHER SOURCE(S): MARPAT 117:131223
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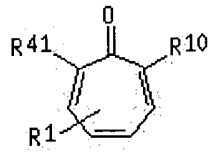

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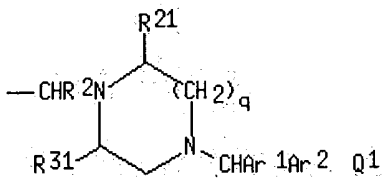

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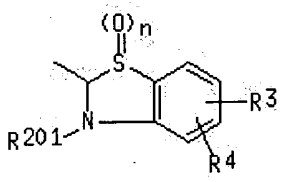

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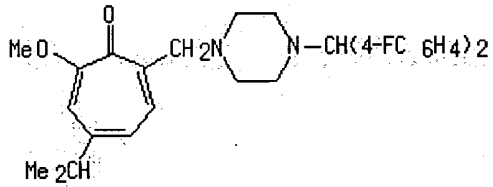


II

AB Title compds. I [R10 = Q1, Q2; R1, R2 = H, C1-5 alkyl, (substituted) aryl, (substituted) hetercyclyl; R3, R4 = H, (substituted) C1-5 alkyl, C7-20 aralkyl, C7-20 aralkyl contg. O, S, or N atoms; halo, OH, C1-5 alkoxy, cyano, etc.; R41 = OR3, OR6, NR7R8, etc.; R6 = H, (substituted) C1-5 alkyl, etc.; R7, R8 = H, (substituted) C1-5 alkyl, C7-20 aralkyl which may contain O, S, or N atoms; NR7R8 = 5-7 membered ring which may contain

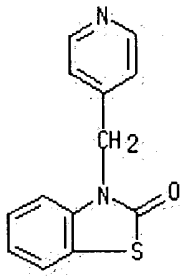
addnl. O or N atoms; R21, R31 = H, C1-3 alkyl; R201 = H, C1-5 alkyl, C2-20 aralkyl, C6-10 arylsulfonyl, C6-10 arylsulfonyl contg. O, S, or N atoms; Ar1, Ar2 = (substituted) aryl; n = 0-2; q = 1-2], were prepd. Thus, a soln. of 7-chloromethyl-4-isopropyl-2-methoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one (prepn. given), 1-(4,4'-difluorobenzhydryl)piperazine, and Et3N in CHCl3 was refluxed for 20 h to give title compd. II. II had minimal ED of <5 mg/kg i.v. in a ischemic heart/reperfusion test in rats.

IT **142224-26-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for ischemia inhibitors)

RN 142224-26-8 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1987:84351 HCAPLUS
DOCUMENT NUMBER:	106:84351
TITLE:	2-(4-Pyridyl)ethyl as a protective group for sulfur functionality
AUTHOR(S):	Katritzky, Alan R.; Takahashi, Ichiro; Marson, Charles M.
CORPORATE SOURCE:	Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SOURCE:	Journal of Organic Chemistry (1986), 51(25), 4914-20 CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 106:84351

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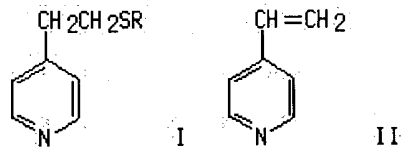


I II

AB 2-(4-Pyridyl)ethyl sulfides I (R = octyl, 2-naphthyl, Ph) were prepd. by Michael addn. of 4-vinylpyridine (II) with thiols RSH, whereas I [R = 5-nitro-2-pyridyl, CH2Ph, Bu, Bz, (PhS)CO] were prepd. by alkylation of thiol I (R = H) with RX (X = halide). I (R = CH2Ph) was also prepd. by alkylation of PhCH2SH with halide I (R = Cl). These sulfides and their corresponding sulfoxides and sulfones were depyridylethylated by quaternization and subsequent treatment with mild base to give the corresponding thiols, sulfinic acids, sulfonic acids, and sulfenamides. During one of these protection-deprotection sequences, Me 1-octyl sulfoxide was readily converted by aerial oxidn. into the corresponding

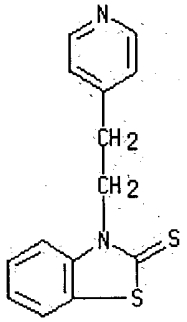
sulfone.

IT **27410-87-3**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with vinylpyridine)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:87880 HCAPLUS
DOCUMENT NUMBER: 74:87880
TITLE: Michael and Mannich reactions with benzothiazole-2-thiol
AUTHOR(S): Halasa, Adel F.; Smith, George E. P., Jr.
CORPORATE SOURCE: Cent. Res. Lab., Firestone Tire and Rubber Co., Akron, OH, USA
SOURCE: Journal of Organic Chemistry (1971), 36(5), 636-41
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

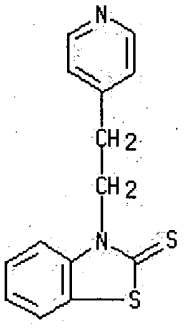
AB The reaction of the anion of benzothiazole-2-thiol (MBT) with activated olefins in the presence of NaH with Michael reaction acceptors produced 3-substituted benzothiazoline-2-thiones. Similarly, the Mannich reaction of MBT anion with HCHO and primary or secondary amines produced the N- (or 3-) substituted benzothiazoline-2-thiones. Possible mechanisms and supporting NMR, ir, and uv data are discussed. The N substitution of MBT anion is discussed within the framework of the oxibase scale which can predict the condition for formation of N products or S products from this ambident anion.

IT **27410-87-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:53769 HCAPLUS
DOCUMENT NUMBER: 74:53769
TITLE: 3-Substituted-2-benzothiazolinethiones
INVENTOR(S): Halasa, Adel F.
PATENT ASSIGNEE(S): Firestone Tire and Rubber Co.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3538109	A	19701103	US 1967-655761	19670725

PRIORITY APPLN. INFO.: US 1967-655761 19670725

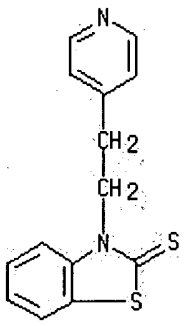
GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are all delayed-action rubber accelerators produced by Michael addns. to benzothiazoline-2-thione (II). Thus, II in freshly distd. THF stirred 48 hr with 4-vinylpyridine and NaH gave I (X = H, Y = 4-pyridyl), m. 159-61°. The corresponding I (X = H, Y = 2-pyridyl), m. 94-5° (alc.), was produced similarly. Analogous reaction of EtCH(NO2)CH2OAc with II give I (X = NO2, Y = Et), m. 89-90°. Similar Michael condensation of BzCH2CH2Cl with II yielded I (X = H, Y = Bz), m. 144.5-5.0° (CHCl3-EtOH).

IT **27410-87-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



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CA SUBSCRIBER PRICE                                        -5.54      -5.54

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

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L3           45 S L1 FULL

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L5            1 S L4 AND ROCHER, J?/AU
L6            1 S L4 AND YAMABE, H?/AU
L7            0 S L6 NOT L5
L8            1 S L4 AND CHAKI, H?/AU
L9            0 S L8 NOT L6
L10           1 S L4 AND ABE, M?/AU
L11           0 S L10 NOT L6
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FILE 'BEILSTEIN' ENTERED AT 15:27:52 ON 09 APR 2004
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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.
 FILE CONTAINS  8,932,479 SUBSTANCES

>>> PLEASE NOTE: Reaction data and substance data are stored in
    separate documents and can not be searched together in one
    query.
    Reaction data for BEILSTEIN compounds may be displayed
    immediately with the display codes PRE (preparations) and REA
    (reactions). A substance answer set retrieved after the search
    for a chemical name, a molecular formula or a structure search
    for example can be restricted to compounds with available
    reaction information by concatenation with PRE/FA, REA/FA or
    more general with RX/FA. The BEILSTEIN Registry Number (BRN)
    is the link between a BEILSTEIN compound and belonging reactions.
    For more detailed reaction searches BRNs can be selected from
    substance answer sets and searched in the next step as reaction
    partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).
    After a search for reaction details substance documents
    associated with reactants or products may be retrieved by
    searching RX.PBRNs or RX.RBRNs as BRNs. <<<


>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

*********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.               *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
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L6            1 S L4 AND YAMABE, H?/AU
L7            0 S L6 NOT L5
L8            1 S L4 AND CHAKI, H?/AU
L9            0 S L8 NOT L6
L10           1 S L4 AND ABE, M?/AU
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L15             1 L3

=> d l15
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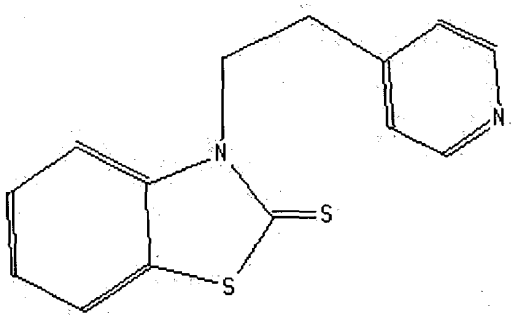
L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1217129
Beilstein Pref. RN (BPR):	27410-87-3
CAS Reg. No. (RN):	**27410-87-3**
Chemical Name (CN):	3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione
Autonom Name (AUN):	3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione
Molec. Formula (MF):	C14 H12 N2 S2
Molecular Weight (MW):	272.38
Lawson Number (LN):	31156, 27396
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1157666
Tautomer ID (TAUTID):	1192884
Beilstein Citation (BSO):	5-27, 6-27
Entry Date (DED):	1988/11/29
Update Date (DUPD):	1993/02/15



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BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	2
MP	Melting Point	4
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXPRO	Substance is Reaction Product	3

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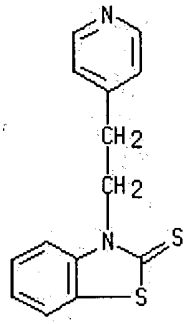
FILE 'REGISTRY' ENTERED AT 15:28:21 ON 09 APR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 27410-87-3 REGISTRY
CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Benzothiazolinethione, 3-[2-(4-pyridyl)ethyl]- (8CI)
FS 3D CONCORD
MF C14 H12 N2 S2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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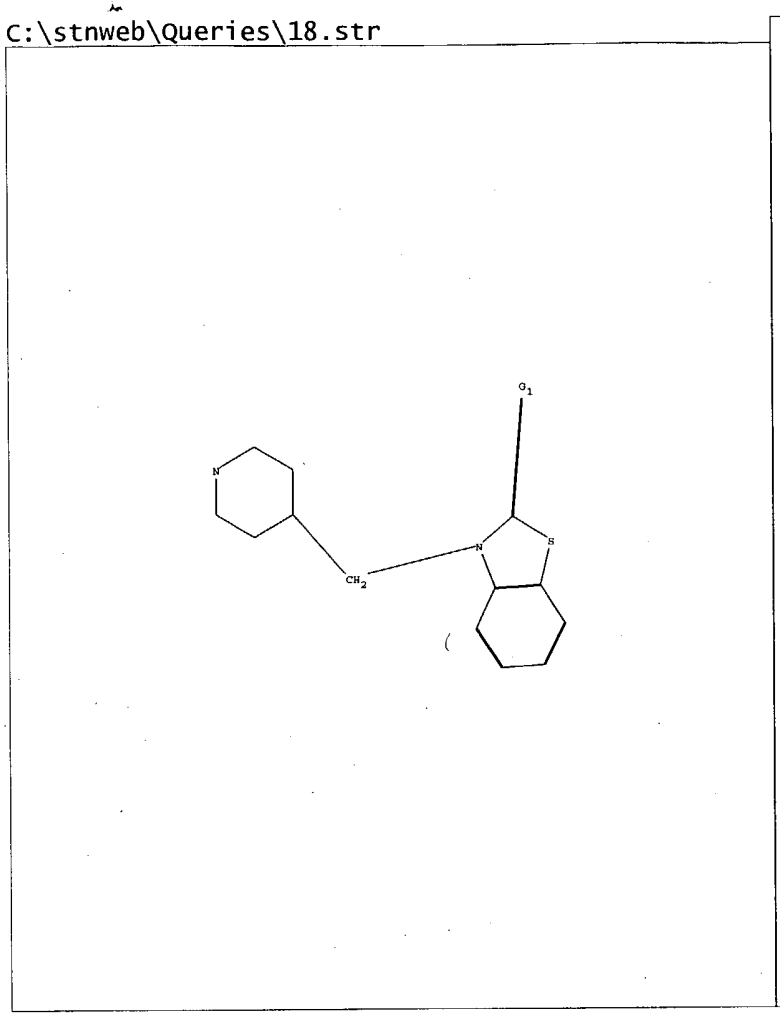

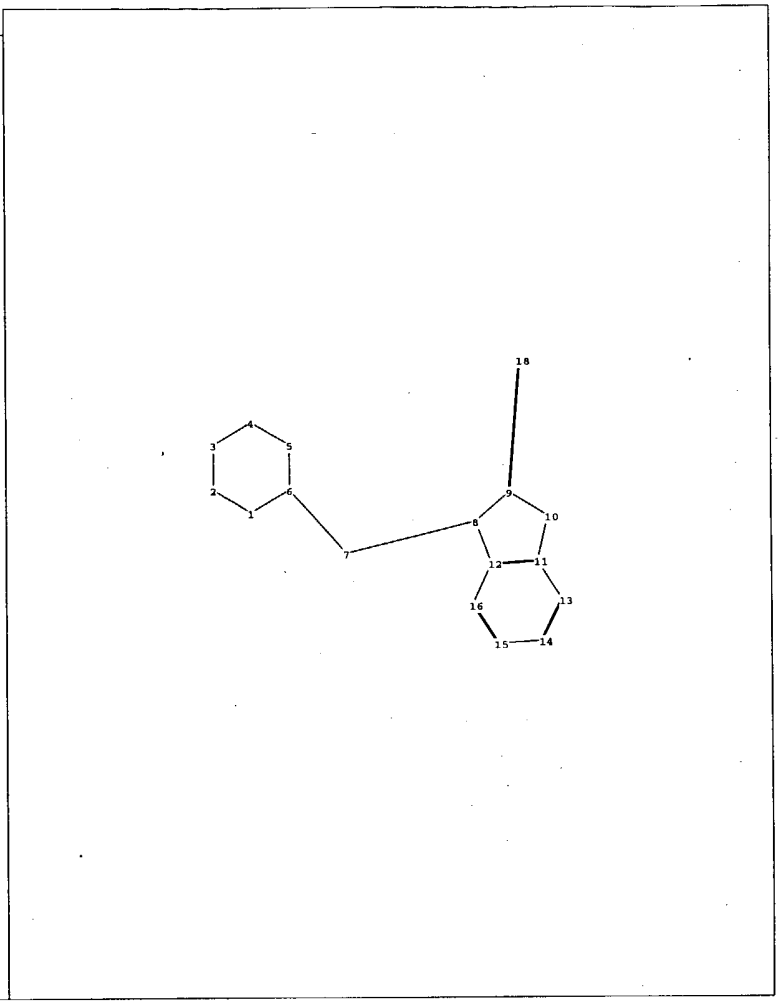

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isolated ring systems :
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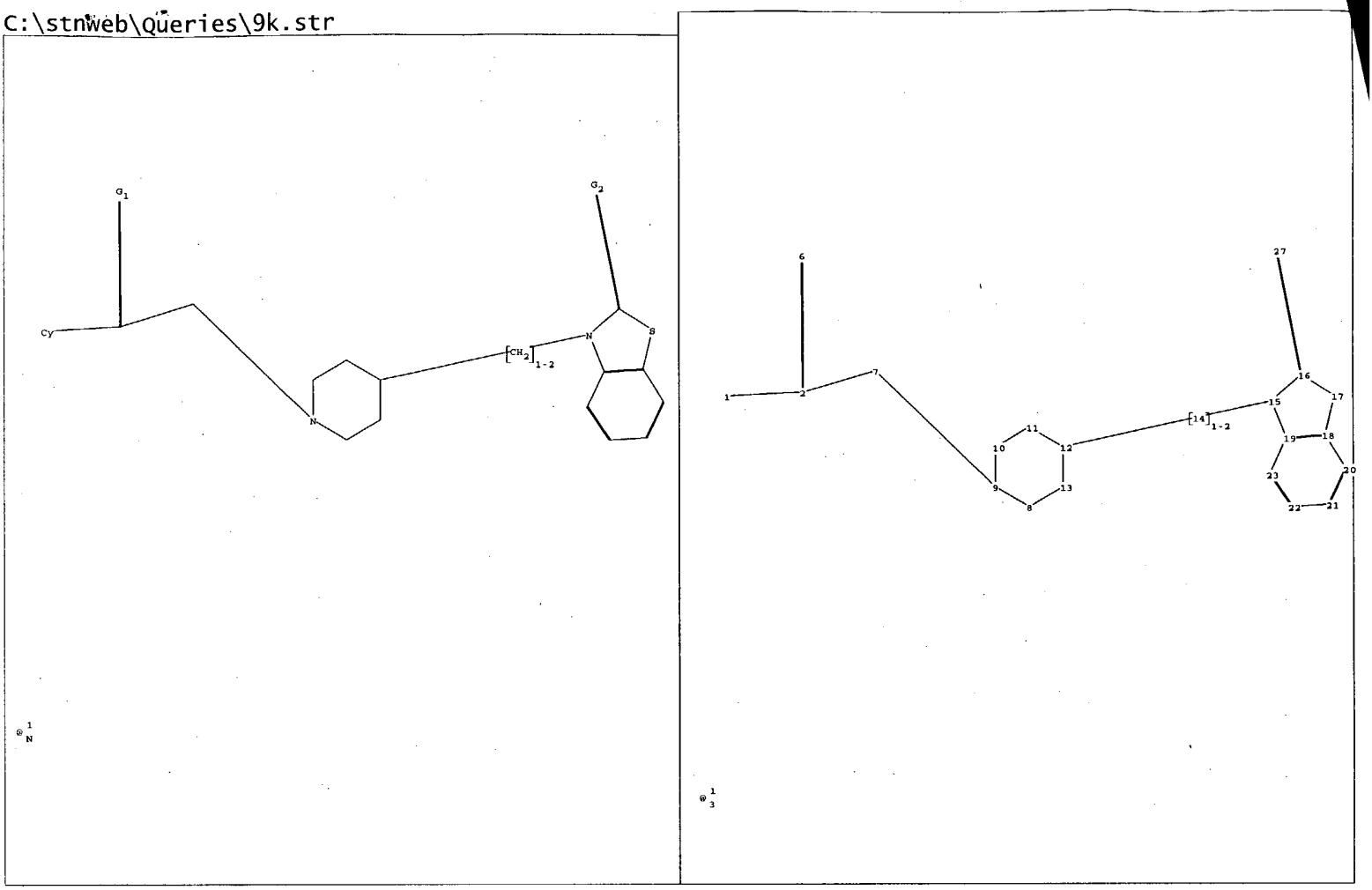

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20-21 21-22 22-23
exact/norm bonds :
1-2 2-6 7-9 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-19 16-27
exact bonds :
2-7 12-14 14-15 16-17 17-18
normalized bonds :
18-19 18-20 19-23 20-21 21-22 22-23
isolated ring systems :
containing 8 : 15 :

G1:O,[*1]

G2:O,S

Match level :
1:Atom 2:CLASS 3:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 27:CLASS

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  NOV 24   MSDS-CCOHS file reloaded
 NEWS  4  DEC 08   CABA reloaded with left truncation
 NEWS  5  DEC 08   IMS file names changed
 NEWS  6  DEC 17   DGENE: Two new display fields added
 NEWS  7  DEC 18   BIOTECHNO no longer updated
 NEWS  8  DEC 19   CROPU no longer updated; subscriber discount no longer
                   available
 NEWS  9  DEC 22   ABI-INFORM now available on STN
 NEWS 10  JAN 27   Source of Registration (SR) information in REGISTRY updated
                   and searchable
 NEWS 11  JAN 27   A new search aid, the Company Name Thesaurus, available in
                   CA/CAplus
 NEWS 12  FEB 05   German (DE) application and patent publication number format
                   changes
 NEWS 13  MAR 03   MEDLINE and LMEDLINE reloaded
 NEWS 14  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS 15  MAR 03   FRANCEPAT now available on STN
 NEWS 16  MAR 29   Pharmaceutical Substances (PS) now available on STN
 NEWS 17  MAR 29   WPIFV now available on STN
 NEWS 18  MAR 29   No connect hour charges in WPIFV until May 1, 2004
 NEWS 19  MAR 29   New monthly current-awareness alert (SDI) frequency in RAPRA

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 14:11:42 ON 09 APR 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 14:11:48 ON 09 APR 2004
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```

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7
DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> **d l1**
L1 HAS NO ANSWERS
L1 STR

=> **s l1**
SAMPLE SEARCH INITIATED 14:13:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> **s l1 full**
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:**y**
FULL SEARCH INITIATED 14:13:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> **file hcaplus**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	156.26	156.47

FILE 'HCAPLUS' ENTERED AT 14:13:38 ON 09 APR 2004
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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d l4, ibib abs fhitstr, 1

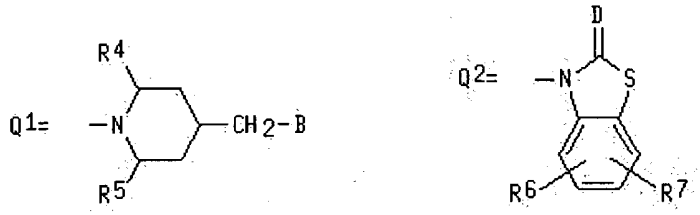
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607 A	19971105
			WO 1998-JP4973 W	19981104

OTHER SOURCE(S): MARPAT 130:338102
GI



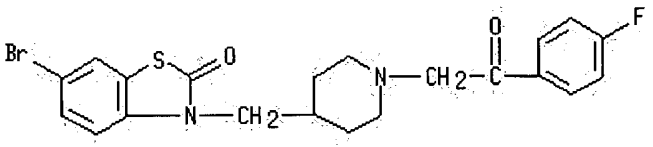
AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-05-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> **file caold**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.12	163.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-0.69

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> **d his**

(FILE 'HOME' ENTERED AT 14:11:42 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 14:11:48 ON 09 APR 2004
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 18 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:38 ON 09 APR 2004
L4 1 S L3

FILE 'CAOLD' ENTERED AT 14:13:48 ON 09 APR 2004

=> **s l3**
L5 0 L3

=> **file beilstein**

COST IN U.S. DOLLARS	SINCE FILE	TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	0.42	164.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.69

FILE 'BEILSTEIN' ENTERED AT 14:13:56 ON 09 APR 2004

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.
FILE CONTAINS 8,932,479 SUBSTANCES

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
**********************************************************************
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=> **s l3**
L6 0 L3

=> **log y**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	164.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.69

STN INTERNATIONAL LOGOFF AT 14:14:06 ON 09 APR 2004